

NASA TECH BRIEF

NASA Pasadena Office



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Three Bit Mass Spectral Search Program

The problem:

The general area of automated spectral analysis is currently very active. There is an ever increasing need for faster and better ways of "interpreting" spectral data.

The solution:

A computer program was developed to "interpret" spectral data in order to assist the chemist in identifying low resolution mass spectra.

How it's done:

A library search against a file of 6880 mass spectra is performed by the computer in order to help identify low resolution mass spectra. For each unknown spectrum, the program provides a list of ten compounds in the library whose spectra are "closest" to the unknown by some goodness-of-fit criterion.

Extensive testing of the program has shown it to be highly reliable and extremely rapid for pure compound and binary mixture identification.

In the 3-bit library search, the peak heights of both the unknown mass spectrum and the library spectrum are encoded to 3 bits, or 8 levels. At each nominal mass, the peak height is an integer I , where $0 < I < 7$. The transitions between levels have been set logarithmically as a function of the percent total ion current. The maximum mass range covered in the search is 12 to 243 amu. By means of data input, narrower mass ranges can be searched. Also, by relatively simple coding changes, it is possible to mask out certain masses or mass number ranges in the search.

Two versions of the program, using approximately the same amount of core are available:

- (a) Up to 30 unknowns per pass through the library can be handled. No detailed side-by-side spectral summary is provided.
- (b) Up to 20 unknowns per pass can be handled. A detailed side-by-side spectral summary is provided at the conclusion of the program.

In both programs, core requirements are roughly proportional to the maximum number of unknowns to be handled on each pass through the tape.

Notes:

1. This program is written in FORTRAN IV (98%) and ASSEMBLER (2%) languages to be utilized on the IBM-360/44 computer. It occupies 128 K bytes of core storage.
2. Inquiries concerning this program should be submitted to:

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